NUCL SCI TECH (2021) 32:119
https://doi.org/10.1007/s41365-021-00971-2

Low-energy atomic displacement model of SRIM simulations

Sheng-Li Chen[1]

Received: 28 August 2021 / Revised: 4 October 2021 / Accepted: 11 October 2021 / Published online: 16 November 2021

Abstract Radiation-induced atomic displacement damage is a pressing issue for materials. The present work investigates the number of atomic displacements using the Primary Knock-on Atom (PKA) energy E_{PKA} and threshold displacement energy E_d as two major parameters via low-energy SRIM Binary Collision Approximation (BCA) full cascade simulations. It is found that the number of atomic displacements cannot be uniquely determined by E_{PKA}/E_d or E_D/E_d (E_D refers to the damage energy) when the energy is comparable with E_d. The effective energy $E_{D,eff}$ proposed in the present work allows to describing the number of atomic displacements for most presently studied monatomic materials by the unique variable $E_{D,eff}/E_d$. Nevertheless, it is noteworthy that the BCA simulation damage energy depends on E_d, whereas the currently used analytical method is independent of E_d. A more accurate analytical damage energy function should be determined by including the dependence on E_d.

Keywords Atomic displacement · Damage energy · Effective energy · SRIM neutron cascade simulations

1 Introduction

Radiation damage is an important issue for materials because it changes the properties of materials (e.g., radiation-induced segregation, swelling, hardening, and variation of resistivity [1]). Primary radiation damage, widely known as atomic displacement damage, is fundamental for studying the irradiation effect on materials. The number of atomic Displacements per Atom (DPA) was proposed to unify the damage caused by different irradiation sources, such as neutrons, protons, photons, electrons, positrons, and ions. DPA is now used as an essential parameter for studying the secondary (or macroscopic) radiation damage of materials [2].

In the past decades, various methods and computational codes have been developed to calculate the number of stable atomic displacements (i.e., Frenkel pairs). The Stopping and Range of Ions in Matter (SRIM) Monte Carlo code [3] (or the former TRansport of Ions in Matter (TRIM) code [4] included in) is widely used for computing atomic vacancies because of its ease of use with a user-friendly graphical interface. Presently, it is almost a non-official standard step to use SRIM simulations for ion irradiation studies.

Regardless of the discrepancy between the Quick Calculation (QC) and Full-Cascade simulations (FC) [5, 6], SRIM is powerful for modeling ion irradiation in materials. However, it cannot be directly used to compute the displacement damage induced by other radiation sources. To unify the atomic vacancies induced by irradiation with different sources, simulation tools or models using the kinetic energy of the Primary Knock-on Atom (PKA) as a major parameter should be used. Therefore, the so-called neutron cascade simulation has been implemented in the

This work was supported by the Fundamental Research Funds for the Central Universities, Sun Yat-sen University (No. 2021qntd12).

✉ Sheng-Li Chen
chenshli23@mail.sysu.edu.cn

[1] Sino-French Institute of Nuclear Engineering and Technology, Sun Yat-Sen University, Zhuhai 519082, China

SRIM code [3]. With the neutron cascade option, users identify the position and energy of PKA in a separate file (i.e., TRIM.DAT) to compute the atomic vacancies induced by a PKA rather than an external ion. For irradiation sources other than ions, the PKA spectra can be determined using specific calculation tools and combined with neutron cascade simulations to obtain the number of point defects. Therefore, consistent results can be obtained for the number of atomic vacancies induced by different irradiation sources with SRIM simulations.

However, the numbers of atomic vacancies (from vacancies.txt file) obtained using the two basic options, QC and FC, of SRIM-like codes differ by a factor of about 2 [5, 6] (1.0–2.7 depending on the incident ion and target atom [7]). Stoller et al. [6] recommended the use of the QC option for obtaining results comparable with the Norgett-Robinson-Torrens (NRT) [8] model. Recently, Crocombette and Van Wambeke [9] and Weber and Zhang [10] recommended using the FC option, especially for compound materials, because it is physically more reasonable. Weber and Zhang [10] and Chen and Bernard [11] explained that the discrepancy between QC and FC is due to the displacements induced by low-energy atoms, which are considered unable to produce additional displacements in classical models [12, 13] (details are given in Sect. 2.1). Nevertheless, the residual energy transfer effect [11] is not evident for a low initial energy. Consequently, further studies on the atomic displacement model for low PKA energy are crucial for unifying the displacement damage induced by different radiation sources, especially for light particles such as electrons, positrons, and photons.

In addition, because the atomic displacements at low energies have an integrated effect on the model at high energies [10], studies on low-energy cascades can reveal the features of the primary radiation damage over the entire energy range. Therefore, the present work investigates the atomic displacements mainly based on SRIM-2013 FC simulations at low PKA energies. The simulation methods are described in Sect. 2.2. The simulated results and corresponding discussion are presented in Sect. 3. Detailed discussion and comments on the use of damage energy for quantifying displacement damage are presented in Sect. 4. The main conclusions of the present study are summarized in Sect. 5.

2 Current atomic displacement models and SRIM simulations

2.1 Current atomic displacement models

The Threshold Displacement Energy (TDE) is defined as the minimum recoil energy required to create a stable point defect. The direction-averaged TDE, denoted by E_d in the present study, is widely used in analytical atomic displacement models. Using E_d, Kinchin and Pease (KP) got a formula for computing the number of atomic vacancies (denoted by ν in the present work) induced by a PKA with the kinetic energy of E_{PKA} as [12]

$$\nu_{KP}(E_{PKA}) = \begin{cases} 0, & E_{PKA} < E_d \\ 1, & E_d \le E_{PKA} < 2E_d \\ \dfrac{E_{PKA}}{2E_d}, & 2E_d \le E_{PKA} < E_c \\ \dfrac{E_c}{2E_d}, & E_{PKA} > E_c. \end{cases} \quad (1)$$

It is noteworthy that the cut-off energy E_c is not used in more recent models nor in the present work. The main reason for this can be found in Ref. [14].

Considering electronic energy loss and a more realistic atomic collision cross section, Norgett, Robinson, and Torrens (NRT) proposed a modified KP formula based on several Binary Collision Approximation (BCA) calculations [8, 15]:

$$\nu_{NRT}(E_D) = \begin{cases} 0, & E_D < E_d \\ 1, & E_d \le E_D < 2E_d/0.8 \\ \dfrac{0.8E_D}{2E_d}, & E_D > 2E_d/0.8, \end{cases} \quad (2)$$

where E_D is the effective energy for atomic motion, also called damage energy, first proposed by Lindhard et al. [16]. Figure 1 shows Lindhard's partition function (i.e., $P = E_D/E_{PKA}$) with Robinson's analytical fitting [17] for various monatomic materials.

Because some displaced atoms are recombined before reaching thermal equilibrium, the Athermal Recombination-Corrected (ARC) model corrects the NRT model for $E_D > 2E_d/0.8 = 2.5E_d$ [13, 18, 19]. The athermal recombination of displaced atoms cannot be simulated by BCA

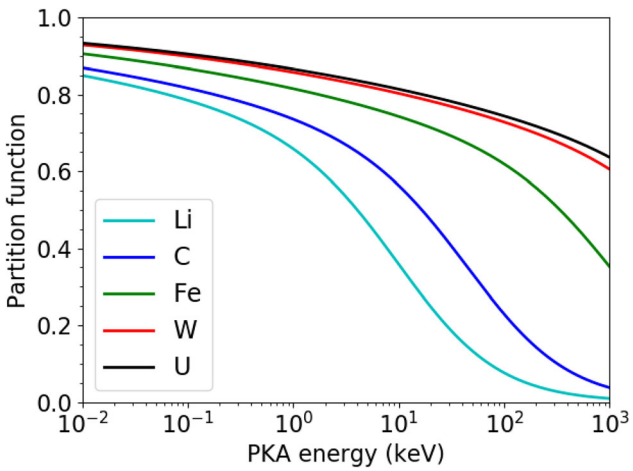

Fig. 1 (Color online) Lindhard's partition function for selected monatomic materials

codes. However, it has a quite limited influence for the low PKA energy, which is the case for the present work; thus, it is not considered here.

In the KP and NRT (or NRT-based) models, one can conclude that the effective variables are E_{PKA}/E_d and E_D/E_d, respectively. Therefore, the present study uses the energy normalized by E_d as an essential parameter to reduce the number of variables and simplify the comparison among different materials as well as the analysis. To simplify the expressions in the following discussion, let $\hat{\nu}$ denote the number of atomic vacancies using the normalized energy as a unique parameter, i.e., $\hat{\nu}_{KP}(E_{PKA}/E_d) = \nu_{KP}(E_{PKA})$ and $\hat{\nu}_{NRT}(E_D/E_d) = \nu_{NRT}(E_D)$.

2.2 SRIM simulations

In SRIM-like codes, there are four methods to obtain the number of atomic displacements: number of vacancies directly from BCA simulations (vacancies.txt for SRIM) and the value calculated using the NRT formula with the damage energy from the BCA simulations for both the QC and FC options. Since the FC option is more physically reasonable, the present work is based on FC.

Because the method of using damage energy is based on the NRT formula, the direct results from collision simulations should be more reliable. Conversely, Agarwal et al. [7] recently pointed out that the latter should be incorrect according to the details of collisions and recommended using the former method. Their reasoning is absolutely convincing. It is however surprising that the results obtained with the recently developed code Iradina are consistent with those of the SRIM FC [9, 20]. In addition, because the first method using damage energy is slightly different from the NRT model calculations, and the theories behind it are well understood, the present work investigates the number of atomic vacancies from SRIM-2013 FC using the vacancies.txt file, simply referred to as SRIM FC hereinafter.

In both the KP and NRT or most other models, it is a common conclusion or assumption that only one atomic vacancy is produced for PKA energy (or damage energy) larger than E_d but smaller than $\sim 2E_d$. For a high initial energy, the atomic displacements induced by a PKA or an incident self-ion are almost identical [11]. For an initial energy comparable with E_d, a PKA is very different from an incident self-ion. Therefore, PKAs, rather than externally incident ions in SRIM simulations, are used in the present work. The original position of the PKAs is set to the center of a $10 \times 10 \times 10$ nm^3 (or larger for a few high PKA energies) cube.

Because SRIM is a stochastic code, the convergence of the Monte Carlo simulations must be ensured. Figure 2 displays the number of atomic vacancies from the SRIM FC of the neutron cascade for 50 and 80 eV Fe PKAs in pure Fe. The study of the numerical convergence is performed on the grid of 2^n PKAs. One can conclude that 8192 (= 2^{13}) PKAs are reasonable to ensure the convergence of SRIM Monte Carlo simulations; thus, the following studies are based on 8192 PKAs simulations. Different from the assumption that $\nu = 1$ for $E_d \leq E_{PKA} < 2E_d$, the SRIM FC gives $\nu > 1$ for $E_d < E_{PKA} < 2E_d$, which is achievable for atomistic simulations because the TDE is direction-dependent. It is much less evident in SRIM simulations owing to the amorphism of the materials. Nevertheless, this is consistent with the case of Ni studied by Weber and Zhang [10]. Agarwal et al. [7] believed that this is due to the incorrect count of some replacements as displacements.

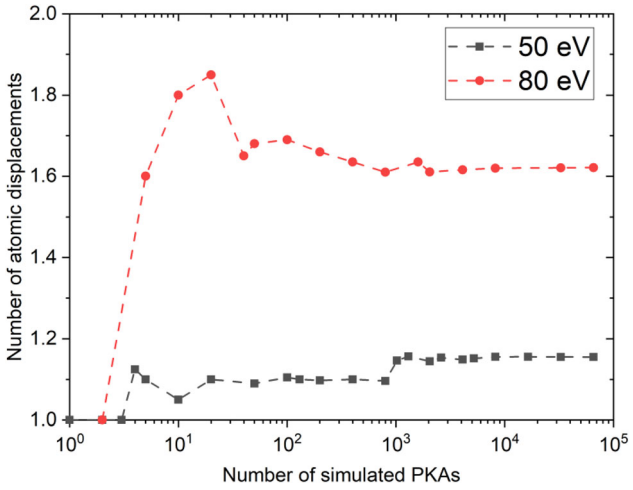

Fig. 2 Number of atomic vacancies in Fe versus the number of simulated PKAs for 50 and 80 eV Fe PKAs

Using SRIM FC, we again compare the displacement damage induced by a PKA and an externally incident ion. Figure 3 plots the number of atomic displacements in Si induced by PKAs and externally incident Si ions (coming from one side of the simulated cube) using the initial kinetic energy and corresponding damage energy as variables. It should be noted that the PKA-induced damage energies used in the present work are the PKA energies after subtracting the ionization energies stored in the IONIZ.TXT SRIM output file. SRIM FC confirms the non-negligible differences between the atomic displacements induced by a PKA and those induced by an incident self-ion when the energies are comparable with E_d. Accordingly, the neutron cascade option must be used to study atomic displacements versus PKA energy.

The present work is based on selected important monatomic materials because the current analytical formula is valid only for monatomic materials. Moreover, the materials are chosen to cover a wide range of atomic numbers (from Z = 6 to 74). Fe and Ni are widely used in stainless steel, Al is used in many fission reactors [21], C,

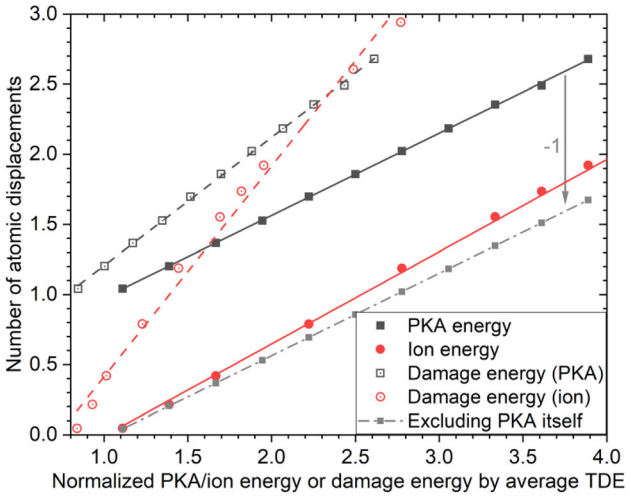

Fig. 3 Number of atomic vacancies in Si versus the PKA (black) or incident ion (red) energy (solid symbols fitted by solid lines) and the corresponding damage energy (center-dotted symbols fitted by dashed lines) with the unit of E_d. The grey plot is the linear fitting of the vacancies versus PKA energy without PKA itself (i.e., –1), it is shown for an intuitive comparison with the vacancies induced by an incident ion

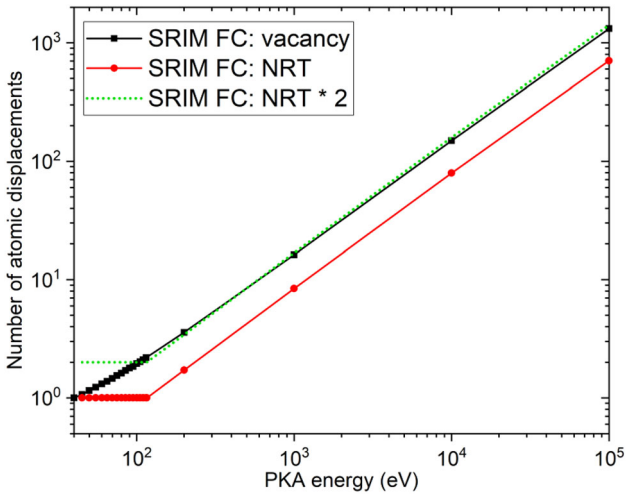

Fig. 4 (Color online) Number of atomic displacements versus PKA energy for Fe PKA in Fe. Vacancy is the data taken from VACANCY.TXT, whereas NRT refers to the value computed with the NRT model using damage energy computed using SRIM FC

Cu, and W [22] are used for fusion applications, and Si is a necessary element for semiconductors in various applications [23]. The average TDEs of the studied elements are given in Table 1. All binding energies are set to be 0 to study the analytical atomic displacement models.

3 Simulation results and discussion

3.1 Atomic displacements from SRIM FC

Figure 4 shows the number of atomic displacements for Fe PKA (i.e., using the neutron cascade option) up to 100 keV in pure Fe by SRIM FC. Both the values from the VACANCY.TXT file and those computed with the NRT formula using the damage energy from the SRM FC are illustrated. The NRT formula is also multiplied by a factor of 2 for an intuitive comparison. The results are quite similar to the case of Ni PKA in Ni shown by Weber and Zhang [10]. For damage energy above $2.5E_d$, a typical discrepancy of a factor of about 2 is found between the SRIM FC and NRT calculation. Such discrepancy has been widely recognized and analyzed [5, 6, 9–11]; therefore, the present work does not emphasize this point.

In the range of $E_d \leq E_D < 2.5E_d$, SRIM FC show that $\nu > 1$ and is a strictly increasing function of damage energy, whereas the NRT model implies that $\nu_{NRT} = 1$. The ratio of SRIM FC to NRT increases from $\sim$ 1 to $\sim$ 2 when E_D increases from $\sim E_d$ to $2.5E_d$. This region has received much less attention because it is not crucial for the displacement damage induced by reactor neutrons and ions. However, it has a large influence on that induced by light particles (e.g., electrons, positrons, photons) (see Refs. [28, 29] for example). Therefore, the atomic displacements for energy below $2.5E_d$ are yet to be studied.

3.2 Atomic displacements for $E_D < E_d$

As the results shown in Fig. 3, atomic displacements are observed when $E_D < E_d$ but $E_{PKA} \geq E_d$. This is a direct consequence of the definition of E_d: a PKA with $E_{PKA} \geq E_d$ is able to produce one atomic displacement (itself or a replacement) because the energy loss in inelastic collisions occurs after the displacement of PKA [29]. Therefore, for PKA energy comparable with E_d, it is questionable to use the damage energy as the effective energy for computing the number of atomic displacements.

The author has proposed a simple modification of the NRT (mNRT) model by assuming that $\nu = 1$ when $(E_{PKA} \geq E_d)\&(E_D < E_d)$ [29]. This modification has a limited influence on the quantification of the primary

Table 1 Average TDE for monatomic materials

Element	C	Al	Si	Fe	Ni	Cu	W
Atomic number	6	13	14	26	28	29	74
E_d (eV)	25 [24]	27 [25]	36 [26]	40 [27]	40 [27]	30 [27]	90 [27]

damage induced by neutron and ions irradiations, of which the contribution of high-energy PKA is predominant. However, its influence on the displacement damage induced by light particles can be considerable [29]. Compared with the original NRT model, the mNRT is more consistent with the SRIM simulations for PKA energy in the range of $(E_{PKA} \geq E_d)\&(E_D < E_d)$. Nevertheless, they are identical for $E_D \geq E_d$; thus, the agreement with the SRIM BCA calculations is barely improved in general.

3.3 Atomic displacements between E_d and $2.5E_d$

Once E_{PKA} is larger than 2 times the minimum TDE, denoted by $E_{d,min}$ hereinafter, it is possible to produce two atomic displacements. Because the TDE is direction dependent, it is possible that $\nu > 1$ for $E_d < E_{PKA} < 2E_d$. In fact, for some materials, $E_d > 2E_{d,min}$. For iron, Table 2 reveals that 9 of the 11 interatomic potentials used in Ref. [30] give $E_d > 2E_{d,min}$. Because the NRT model and NRT-based models use $2.5E_d$ as a demarcation energy to ensure continuity, we investigate the point defects for both PKA energy and damage energy in the range of $[E_d, 2.5E_d]$. Because the present work and the SRIM code use only the average TDE, it is simply denoted by TDE hereinafter if without any other statement.

Figure 5 plots the numbers of atomic displacements for various monatomic materials with PKA and damage energies between E_d and $2.5E_d$. For the sake of simplification, they are respectively denoted by $\hat{\nu}_{KP}$ (left plot) and $\hat{\nu}_{NRT}$ (right plot) with the variables E_{PKA}/E_d and E_D/E_d. It is obviously confirmed that $\nu > 1$ for $E_{PKA} > E_d$ for all monatomic materials. Excluding the material dependence already included in E_d (and E_D), $\hat{\nu}$ is additionally dependent on the material. For the seven monatomic materials studied in the present work, Fe, Ni, and Cu follow almost the same law. $\hat{\nu}_{KP}$ of C and W are quasi-identical but smaller than that of the other five. $\hat{\nu}_{KP}$ of Si is between those of Al, Fe, Ni, and Cu and the ones of C and W. However, $\hat{\nu}_{NRT}$. seems to be decreasing with the increasing atomic number of the target. The main reason is that the partition function is larger for heavier atoms [14, 16] (Fig. 1). It is noticeable that. of C and W are quite different, whereas their $\hat{\nu}_{KP}$ are quasi-identical.

The discrepancies shown in Fig. 5 can be attributed to the different materials and different TDEs. Therefore, Fig. 6 compares the results of Si with two different values of E_d. It is noted that 24 eV is the average threshold energy for a bond defect or a Frenkel pair [26]. This value is comparable with $E_d = 21$ eV obtained by Bourgoin et al. [31]. It can bconcluded that the value of E_d influences both $\hat{\nu}_{KP}$ and $\hat{\nu}_{NRT}$, even though they are independent of E_d in typical models (cf. Section 2.1). In addition, comparing the results of C (Fig. 5) and Si (Figs. 5 and 6), $\hat{\nu}_{KP}$ and $\hat{\nu}_{NRT}$ of Si with $E_d = 24$ eV are larger than those of C, of which $E_d = 25$ eV. Consequently, $\hat{\nu} > 1$ for $E_{PKA} > E_d$ and $\hat{\nu}$ depends on both the material and value of E_d. Therefore, we cannot obtain a unique simple function of E_{PKA}/E_d or E_D/E_d to describe the number of atomic displacements from the SRIM FC in the range of $(E_{PKA} \geq E_d)$ and $(E_D < 2.5E_d)$. Nevertheless, as the results shown in Figs. 5 and 6, a linear fitting of the number of atomic displacements vs. PKA energy or damage energy is suitable for each monatomic material.

4 Comments on the effective energy in displacement models

Comparing the two plots with the PKA energy shown in Fig. 6, $E_d = 24$ eV has large number of atomic displacements than $E_d = 36$ eV for a given E_{PKA}/E_d. For a specific material with a smaller E_d, the same E_{PKA}/E_d implies a smaller E_{PKA}, so that the partition function is larger, which further implies a larger E_D/E_d. Therefore, the two different plots versus PKA energy in Fig. 6 confirm that the damage energy better describes the number of atomic displacements than the PKA energy.

However, the results versus damage energy illustrated in Fig. 6 show that the damage energy is not necessarily better than the PKA energy for determining a simple unique formula for a specific material. In fact, the inelastic energy loss has little influence on the atomic displacements when the kinetic energy is comparable with or even smaller than E_d. Therefore, the PKA energy and damage energy are two extreme energies for computing the atomic

Table 2 Comparison of E_d and $E_{d,min}$ for Fe with 11 different potentials [30]

Potential	ERG	ABC	WOL	COWP	MHS	AMS	SP-RB	HA-VD	HV-TB	JO-GA	FS-CB
$E_{d,min}$ (eV)	15	17	21	19	15	15	15	19	17	15	15
E_d (eV)	40	45	41	54	37	39	42	33	46	37	39
$E_d/E_{d,min}$	2.7	2.6	1.9	2.8	2.5	2.6	2.8	1.8	2.7	2.4	2.6

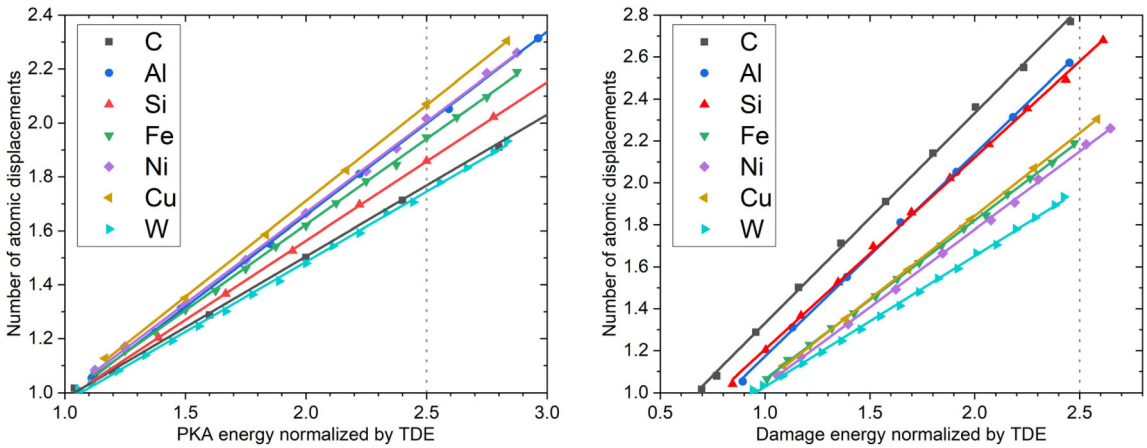

Fig. 5 (Color online) Number of atomic vacancies versus normalized PKA (left, noted by $\hat{\nu}_{\mathrm{KP}}$ in the text) and damage (right, noted by $\hat{\nu}_{\mathrm{NRT}}$ in the text) energies from SRIM FC of neutron cascade. The straight lines are linear fittings

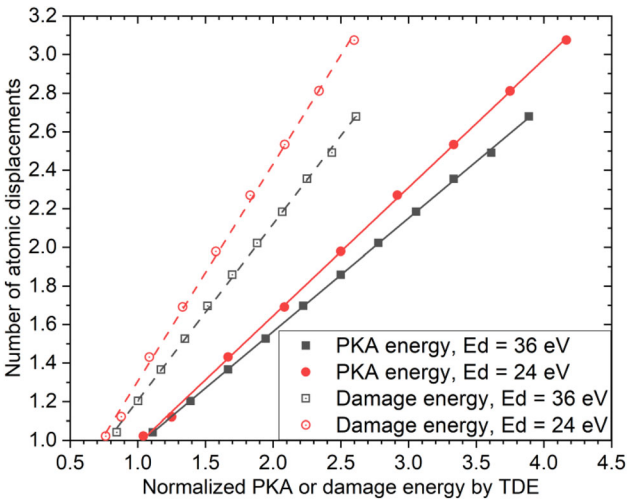

Fig. 6 (Color online) Number of atomic vacancies versus the normalized PKA (solid points) and damage (center-dotted points) energies for Si with E_{d} = 36 eV (black squares) and 24 eV (red circles). The straight lines are linear fittings

displacements. New efficient energy should be determined for more accurate calculations.

4.1 Correcting the damage energy in the displacement calculation

Robinson and Oen [32] recognized that the inelastic energy loss for atoms with kinetic energy smaller than $2.5E_{\mathrm{d}}$ does not influence the number of atomic displacements. Thus, the inelastic energy loss when an atom slows down from $2.5E_{\mathrm{d}}$ to 0 should be added to the damage energy for computing the atomic displacements [32]. Based on this reasoning, they obtained the effective energy as [32]

$$E_{\mathrm{D,eff}}(E_{\mathrm{PKA}}) = \frac{2.5E_{\mathrm{d}}}{E_{\mathrm{D}}(2.5E_{\mathrm{d}})} E_{\mathrm{D}}(E_{\mathrm{PKA}}). \tag{3}$$

It is noteworthy that the demarcation of $2.5E_{\mathrm{d}}$ in the NRT formula is used only to ensure the continuity of the displacement function. According to the reasoning of Kinchin and Pease [12], $2E_{\mathrm{d}}$ is a physically crucial limit. In addition, an atom does not slow down with continuous energy loss. A collision may decrease the energy of an atom from $E_1 > 2E_{\mathrm{d}}$ to $E_2 < 2E_{\mathrm{d}}$. Assuming the equiprobable energy distribution (i.e., hard-sphere collision [11]) for an atom slowed down to $E < 2E_{\mathrm{d}}$ for the first time, one can introduce a correction factor by

$$\eta = \int_0^{2E_{\mathrm{d}}} \frac{E_{\mathrm{PKA}}}{E_{\mathrm{D}}(E_{\mathrm{PKA}})} \mathrm{d}E_{\mathrm{PKA}} \Big/ \int_0^{2E_{\mathrm{d}}} \mathrm{d}E_{\mathrm{PKA}}. \tag{4}$$

Because the partition function can be considered as quasi-constant for the PKA energy from 0 to $2E_{\mathrm{d}}$, $E_{\mathrm{D}}(E_{\mathrm{PKA}}) \approx E_{\mathrm{PKA}} \times P(E_{\mathrm{d}})$ when $0 \le E_{\mathrm{PKA}} \le 2E_{\mathrm{d}}$. Therefore, the correction factor can be approximated using

$$\eta \approx \frac{1}{P(E_{\mathrm{d}})} = \frac{E_{\mathrm{d}}}{E_{\mathrm{D}}(E_{\mathrm{d}})}. \tag{5}$$

Using Lindhard's analytical partition function for monatomic materials, η can be simply calculated as

$$\eta \approx 1 + 0.2161 Z^{5/18} A^{-1/2} E_{\mathrm{d}}^{1/6}. \tag{6}$$

For atoms from Li to U with E_{d} of several tens of eV, $\eta \approx 1.2$. This value is in good agreement with the experimental values of Fe and Ni summarized in the Nuclear Energy Agency (NEA) report [33], the experimental results of Cu obtained by Averback et al. [34], and many MD simulations for energy around $2E_{\mathrm{d}}$.

It is noticeable that the correction factor proposed by Robinson and Oen [32] is numerically close to the present one because the partition function varies insignificantly

between E_d and $2.5E_d$. The difference is only a factor of 1.16 in the second term of η. Therefore, $\eta \approx 1.2$ for both corrections. This value leads to $\nu_{NRT}(E_D) \approx E_D/2E_d$ for $E_D > 2E_d$. One obtains exactly the same formula as the KP formula by replacing of the PKA energy with the damage energy.

However, it is noticeable that $\kappa \approx 0.86$ or 0.8 in the formula $\nu_{NRT}(E_D) = \kappa E_D/2E_d$ is determined by fitting the BCA calculation results [15]. Therefore, if the effective energy $E_{D,eff} = \eta E_D$ rather than E_D is used, the fitted constant (or widely recognized as the correction to the hard-sphere collision cross section) becomes $\kappa' = \kappa/\eta \approx 0.7$.

4.2 Effective energy for SRIM simulations

Because Lindhard's partition function is slightly different from that computed by SRIM, the present correction factor for damage energy is calculated with $E_D(E_d)$ from SRIM FC and denoted by η_{SRIM}. The effective energy is computed as follows:

$$E_{D,eff}(E_{PKA}) = \eta_{SRIM} E_D(E_{PKA}). \quad (7)$$

The results shown in Fig. 5 are rescaled by η_{SRIM} and are illustrated in Fig. 7. Excluding W, the six monatomic materials considered in the present work (from C to Cu) almost follow the same law, which uses $E_{D,eff}/E_d$ as a unique variable. Therefore, this effective energy provides the possibility to correct the current formulae and describe the results of IM FC. Moreover, the use of η. satisfies $\nu(E_{PKA} = E_d) = 1$, which is consistent with the definition of E_d.

The fitted line in Fig. 7 indicates that $\nu_{SRIM} \approx 0.7(E_{D,eff}/E_d - 1) + 1$. Assuming its applicability up to high energies, once $\nu \gg 0.3$, $\nu_{SRIM} \approx 0.7E_{D,eff}/E_d = 0.7\eta_{SRIM}E_D/E_d$. For most cases where $\eta_{SRIM} \approx 1.1$ or 1.2, $\nu_{SRIM} \approx 0.8E_D/E_d = 2\nu_{NRT}$. is relationship explains the typical discrepancy of a factor of about 2 between the SRIM FC and NRT formula.

However, it should be noted that the number of atomic displacements in W still differs from the others. Moreover, the use of η_{SRIM} cannot make the two curves of Si in Fig. 6 coincide. In fact, it is important to indicate that the damage energy from the SRIM FC depends on the value of E_d (e.g., the example on Si shown in Fig. 8), whereas Lindhard's damage energy is independent of E_d [16]. Using the data for $E_d = 36$ eV as a reference, we rescale the effective energy for $E_d = 24$ eV by a factor of 1.1 to get the same damage energy function. The rescaled data are plotted in Fig. 9 together with the data versus the damage energy and effective energy. Rescaling the effective energy to eliminate the bias induced by E_d results in similar atomic displacements for Si with $E_d = 24$ eV and $E_d = 36$ eV.

From the case of Si shown above, one can find that none of $E_{D,eff}/E_d$, E_D/E_d, and E_{PKA}/E_d can be the unique variable for describing the number of atomic displacements from the SRIM FC. Therefore, the number of atomic displacements versus $E_{D,eff}/E_d$, E_D/E_d, or E_{PKA}/E_d for two arbitrary monatomic materials are not necessarily the same. The only general conclusion is that linear fitting can be used to describe the number of atomic displacements versus $E_{D,eff}$, E_D, and E_{PKA} for energy comparable with E_d. One can also adopt a specific value of E_d for W to reduce the difference with the other materials, as shown in Fig. 7. The difference decreases but still exists using of $E_d =$ 55 eV [35, 36] rather than 90 eV. The difference can be

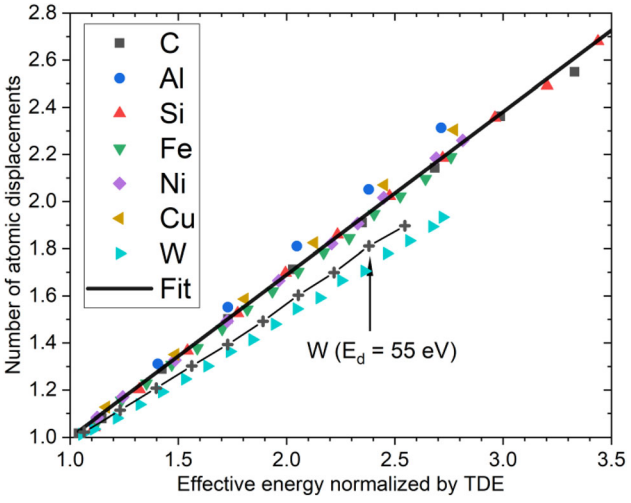

Fig. 7 (Color online) Number of atomic displacements versus the effective energy from the SRIM FC of neutron cascade. The straight line is the linear fitting of the six cases excluding W (R^2 = 0.994)

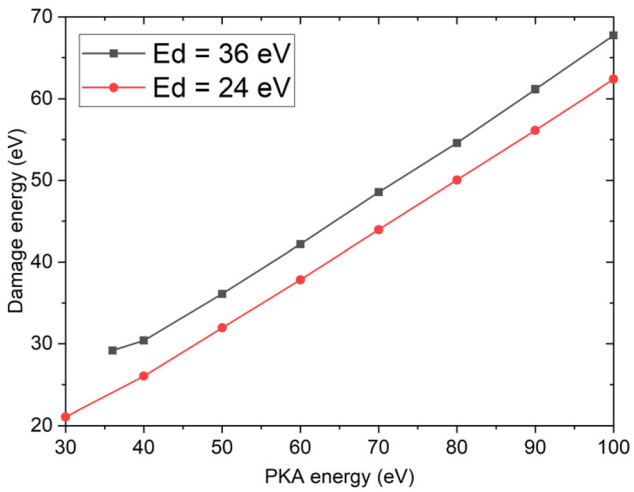

Fig. 8 (Color online) Damage energy versus PKA energy from SRIM-2013 FC for Si with E_d = 36 eV (black) and 24 eV (red)

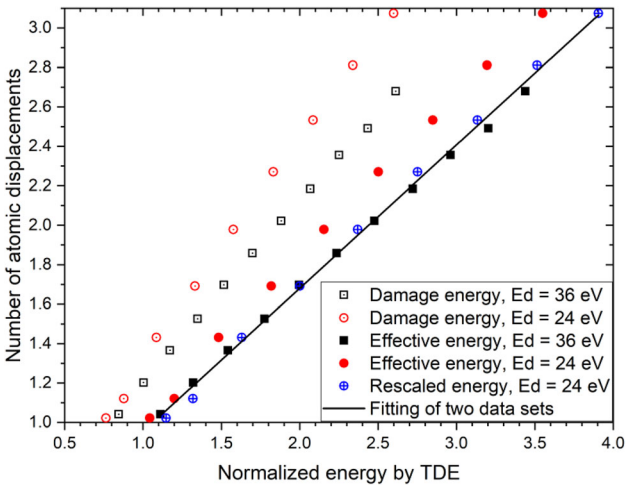

Fig. 9 (Color online) Number of atomic displacements versus the normalized damage and effective energies for Si using E_d = 24 eV (circle) and 36 eV (square). The straight line is the linear fitting of two data sets (R^2 = 0.997)

further decreased by decreasing E_d; however, using an unphysical value for E_d is unnecessary.

4.3 Further comments on the damage energy

Figure 8 shows that the damage energy from SRIM FC depends on the value of E_d, whereas the Lindhard's damage energy is independent of E_d. However, these are not physically incompatible. In fact, the original equation governing the damage energy (or atomic vacancies) includes E_d as a basic parameter [16]. The currently used Lindhard's damage energy is TDE-independent because it is obtained according to the numerical solutions after removing E_d in the original equation (i.e., their approximation (B): E_d is negligeable when compared with kinetic energies of atoms [16]).

Table 3 summarizes the damage energies and numbers of atomic displacements for Fe PKA in Fe from SRIM FC using two different values for E_d: 40 eV and 20 eV. The results show that the damage energy depends on E_d for PKA energies up to 100 keV. For a given PKA energy, the damage energy is larger for a larger E_d. This is a consequence of knocked-on atoms having a smaller kinetic energy for larger E_d. A lower kinetic energy results in lower inelastic energy losses in subsequent collisions. Therefore, once E_d is changed, the corresponding number of atomic displacements cannot be directly predicted as the inverse proportion to E_d. Taking the Fe PKA in Fe shown in Table 3 as an example, the number of atomic displacements is reduced by a factor greater than 2 (the last column in Table 3) if E_d is doubled (20 eV $\rightarrow$ 40 eV), whereas the NRT model predicts a reduction of a factor of 2 (or smaller than 2 if the slight increase in damage energy is considered). This confirms the conclusion given in Sect. 4.2: E_D/E_d or $E_{D,eff}/E_d$ cannot be the unique variable for computing the number of atomic displacements. A variation of E_d by a factor of x does not imply a variation of a factor of $1/x$ for the number of atomic displacements.

5 Conclusion

In SRIM FC, the number of atomic displacements $\nu > 1$ and cannot be uniquely described by E_D/E_d or E_{PKA}/E_d for PKA energy from E_d to a few times of E_d. Because a part of the inelastic energy loss (when the kinetic energy is smaller than $\sim 2E_d$) does not influence the number of atomic displacements, an effective energy $E_{D,eff} = \eta E_D$ is proposed. An approximate value of $\eta \approx 1.2$ is obtained for both the present proposal and that of Robinson and Oen [32]. This value is consistent with the experimental data for Fe, Ni, and Cu for damage energies of about $2E_d$. Using $\eta_{SRIM} = E_d/E_D(E_d)$, six of the seven monatomic materials considered in the present work have the same number of atomic displacements as a function of $E_{D,eff}/E_d$.

However, further investigation shows that the damage energy depends on E_d, whereas the currently used analytical damage energy is independent of E_d. For a given PKA energy, the damage energy is larger for a larger E_d. Consequently, none of $E_{D,eff}/E_d$, E_D/E_d, and E_{PKA}/E_d can be the unique variable for describing the number of atomic displacements. The only general conclusion is that a linear function fitting is suitable for quantifying the number of atomic displacements as a function of $E_{D,eff}$, E_D, and E_{PKA} for energy comparable with E_d. A more accurate analytical

Table 3 Damage energy and the number of atomic displacements for Fe PKA in Fe with E_d = 40 eV (a) and 20 eV (b) from SRIM FC

PKA energy (keV)	Damage energy (keV)			Number of atomic displacements		
	(a)	(b)	(a)/(b)	(a)	(b)	(a)/(b) × 2
0.1	0.0862	0.0819	1.053	1.95	4.09	0.952
1	0.8408	0.7927	1.061	16.2	37.1	0.875
10	7.941	7.466	1.064	149	343	0.871
100	70.65	66.35	1.065	1319	3040	0.867

damage energy function should be determined by solving Lindhard's integro-differential equation with E_d.

References

1. G. S. Was, The Displacement of Atoms. in *Fundamentals of Radiation Materials Science*, New York, NY: Springer New York, pp. 77–130 (2017).
2. ISO 19226:2017, *Nuclear energy—of neutron fluence and displacement per atom (dpa) in reactor vessel and internals*. (2017)
3. J.F. Ziegler, M.D. Ziegler, J.P. Biersack, SRIM – The stopping and range of ions in matter (2010). Nucl. Instrum. Methods Phys. Res. Sect. B **268**(11), 1818–1823 (2010). https://doi.org/10.1016/j.nimb.2010.02.091
4. J.P. Biersack, L.G. Haggmark, A Monte Carlo computer program for the transport of energetic ions in amorphous targets. Nucl. Instrum. Methods. **174**(1), 257–269 (1980). https://doi.org/10.1016/0029-554X(80)90440-1
5. M.I. Bratchenko, V.V. Bryk, S.V. Dyuldya et al., Comments on DPA calculation methods for ion beam driven simulation irradiations. Вопросы Атомной Науки И Техники. **2**(84), 11–16 (2013)
6. R.E. Stoller, M.B. Toloczko, G.S. Was et al., On the use of SRIM for computing radiation damage exposure. Nucl. Instrum. Methods Phys. Res. Sect. B **310**, 75–80 (2013). https://doi.org/10.1016/j.nimb.2013.05.008
7. S. Agarwal, Y. Lin, C. Li et al., On the use of SRIM for calculating vacancy production: Quick calculation and full-cascade options. Nucl. Instrum. Methods Phys. Res. Sect. B **503**, 11–29 (2021). https://doi.org/10.1016/j.nimb.2021.06.018
8. M.J. Norgett, M.T. Robinson, I.M. Torrens, A proposed method of calculating displacement dose rates. Nucl. Eng. Des. **33**(1), 50–54 (1975). https://doi.org/10.1016/0029-5493(75)90035-7
9. J.-P. Crocombette, C. Van Wambeke, Quick calculation of damage for ion irradiation: implementation in Iradina and comparisons to SRIM. EPJ Nucl. Sci. Technol. **5**, 7 (2019). https://doi.org/10.1051/epjn/2019003
10. W.J. Weber, Y. Zhang, Predicting damage production in monoatomic and multi-elemental targets using stopping and range of ions in matter code: challenges and recommendations. Curr. Opin. Solid State Mater. Sci. **23**(4), 100757 (2019). https://doi.org/10.1016/j.cossms.2019.06.001
11. S. Chen, D. Bernard, On the calculation of atomic displacements using damage energy. Results Phys. **16**, 102835 (2020). https://doi.org/10.1016/j.rinp.2019.102835
12. G.H. Kinchin, R.S. Pease, The displacement of atoms in solids by radiation. Rep. Prog. Phys. **18**, 1–51 (1955). https://doi.org/10.1088/0034-4885/18/1/301
13. K. Nordlund, S.J. Zinkle, A.E. Sand et al., Primary radiation damage: a review of current understanding and models. J. Nucl. Mater. **512**, 450–479 (2018). https://doi.org/10.1016/j.jnucmat.2018.10.027
14. S. Chen, D. Bernard, C. De Saint Jean, Relativistic effect on atomic displacement damage for two-body inducing discrete reactions. EPJ Web Conf. **239**, 08004 (2020). https://doi.org/10.1051/epjconf/202023908004
15. M.T. Robinson, I.M. Torrens, Computer simulation of atomic-displacement cascades in solids in the binary-collision approximation. Phys. Rev. B **9**(12), 5008–5024 (1974). https://doi.org/10.1103/PhysRevB.9.5008
16. J. Lindhard, V. Nielsen, M. Scharff, et al., Integral equations governing radiation effects. Mat.-Fys. Meddelelser Konglige Dan. Vidensk. Selsk. **33**(10), 1–42 (1963)
17. M. T. Robinson, The Energy Dependence of Neutron Radiation Damage in Solids. in *Nuclear Fusion Reactors*. 364–378 (1970). Doi: https://doi.org/10.1680/nfr.44661.0025
18. K. Nordlund, S.J. Zinkle, A.E. Sand et al., Improving atomic displacement and replacement calculations with physically realistic damage models. Nat. Commun. **9**(1), 1084 (2018). https://doi.org/10.1038/s41467-018-03415-5
19. AYu. Konobeyev, U. Fischer, S.P. Simakov, Improved atomic displacement cross-sections for proton irradiation of aluminium, iron, copper, and tungsten at energies up to 10 GeV. Nucl. Instrum. Methods Phys. Res. Sect. B **431**, 55–58 (2018). https://doi.org/10.1016/j.nimb.2018.06.021
20. C. Borschel, C. Ronning, Ion beam irradiation of nanostructures—a 3D Monte Carlo simulation code. Nucl. Instrum. Methods Phys. Res. Sect. B **269**(19), 2133–2138 (2011). https://doi.org/10.1016/j.nimb.2011.07.004
21. D. Saad, H. Benkharfia, M. Izerrouken et al., Displacement damage cross section and mechanical properties calculation of an Es-Salam research reactor aluminum vessel. Nucl. Sci. Tech. **28**(11), 162 (2017). https://doi.org/10.1007/s41365-017-0319-3
22. R.A. Pitts, S. Carpentier, F. Escourbiac et al., A full tungsten divertor for ITER: Physics issues and design status. J. Nucl. Mater. **438**, S48–S56 (2013). https://doi.org/10.1016/j.jnucmat.2013.01.008
23. A. Akkerman, J. Barak, M. Murat, A survey of the analytical methods of proton-NIEL calculations in silicon and germanium. IEEE Trans. Nucl. Sci. **67**, 1813–1825 (2020). https://doi.org/10.1109/TNS.2020.2998006
24. A.J. McKenna, T. Trevethan, C.D. Latham et al., Threshold displacement energy and damage function in graphite from molecular dynamics. Carbon **99**, 71–78 (2016). https://doi.org/10.1016/j.carbon.2015.11.040
25. P. Lucasson, The production of frenkel defects in metals. in *Fundamental aspects of radiation damage in metals*, Oak Ridge National Laboratory, US. 1, 42–65 (1975).
26. E. Holmström, A. Kuronen, K. Nordlund, Threshold defect production in silicon determined by density functional theory molecular dynamics simulations. Phys. Rev. B. **78**(4), 045202 (2008). https://doi.org/10.1103/PhysRevB.78.045202
27. ASTM E521-96, Practice for Neutron Radiation Damage Simulation by Charged-Particle Irradiation. ASTM International, West Conshohocken, PA, 1996. https://doi.org/10.1520/E0521-96
28. S. Chen, D. Bernard, C. De Saint Jean, Calculation and analysis of gamma-induced irradiation damage cross section. Nucl. Instrum. Methods Phys. Res. Sect. B. **447**, 8–21 (2019). https://doi.org/10.1016/j.nimb.2019.03.035
29. S. Chen, D. Bernard, On the beta decay-induced radiation damage. Nucl. Instrum. Methods Phys. Res. Sect. B **467**, 58–64 (2020). https://doi.org/10.1016/j.nimb.2020.01.017
30. K. Nordlund, J. Wallenius, L. Malerba, Molecular dynamics simulations of threshold displacement energies in Fe. Nucl. Instrum. Methods Phys. Res. Sect. **246**(2), 322–332 (2006). https://doi.org/10.1016/j.nimb.2006.01.003
31. J.C. Bourgoin, P. Ludeau, B. Massarani, Threshold energy determination in thick semiconductor samples. Rev. Phys. Appl. **11**(2), 279–284 (1976). https://doi.org/10.1051/rphysap:01976001102027900
32. M.T. Robinson, O.S. Oen, On the use of thresholds in damage energy calculations. J. Nucl. Mater. **110**(2), 147–149 (1982). https://doi.org/10.1016/0022-3115(82)90139-8
33. K. Nordlund, A. E. Sand, F. Granberg, *et al.*, Primary Radiation Damage in Materials. OECD/NEA. NEA/NSC/DOC(2015)9

(2015). https://www.oecd-nea.org/science/docs/2015/nsc-doc2015-9.pdf
34. R.S. Averback, R. Benedek, K.L. Merkle, Ion-irradiation studies of the damage function of copper and silver. Phys. Rev. B **18**(8), 4156 (1978). https://doi.org/10.1103/PhysRevB.18.4156
35. F. Maury, M. Biget, P. Vajda et al., Frenkel pair creation and stage I recovery in W crystals irradiated near threshold. Radiat. Eff. **38**(1–2), 53–65 (1978). https://doi.org/10.1080/00337577808233209
36. D.R. Mason, X. Yi, M.A. Kirk et al., Elastic trapping of dislocation loops in cascades in ion-irradiated tungsten foils. J. Phys. Condens. Matter **26**(37), 375701 (2014). https://doi.org/10.1088/0953-8984/26/37/375701